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Magnetic structure of the heavy fermion alloy $CeCu_{5.5}Au_{0.5}$

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Abstract

Neutron diffraction measurements were performed on a single crystal of the heavy fermion compound $CeCu_{5.5}Au_{0.5}$. Below $T_N = 1.00 \pm 0.05$ K an incommensurate magnetic structure was found with wave vector $q = (\pm 0.59, 0, 0)$, which completely explains the previous powder diffraction data. This wave vector differs from the wave vectors characterizing the correlated fluctuations in $CeCu_6$, where q along the a^* direction is commensurate.

The heavy fermion compound $CeCu_6$ does not show any long-range static magnetic order. However, antiferromagnetic and incommensurate correlated fluctuations have been observed by inelastic neutron scattering at low temperatures [1]. On the other hand, long-range magnetic order occurs in the alloy $CeCu_{6-x}Au_x$ for $x > 0.1$ with an ordering temperature T_N which increases with Au concentration up to $x = 1$, as evidenced by sharp maxima in the specific heat and susceptibility [2]. Neutron diffraction on a $CeCu_{5.5}Au_{0.5}$ polycrystal exhibited some magnetic reflections, confirming the long-range nature of this magnetic order [3]. However, the magnetic structure, not being simple antiferromagnetic, could not be resolved. Here we present the first neutron diffraction measurements on a single crystal of $CeCu_{6-x}Au_x$ with $x = 0.5$ to reveal the magnetic structure.

Neutron diffraction measurements were carried out at NIST on BT9 in a double-axis mode using the neutron wavelength $\lambda = 2.3556$ Å with a PG-filter. The two single crystals investigated were part of a big $CeCu_{5.5}Au_{0.5}$ crystal, grown in KFA Jülich, as the samples used for specific heat and magnetization measurements [4]. $CeCu_{5.5}Au_{0.5}$ crystallizes like $CeCu_6$ in the orthorhombic structure Pnma at 300 K [4]. At low temperatures ($T \approx 1$ K) we found the orthorhombic symmetry still present in contrast to $CeCu_6$, which becomes monoclinic below $T < 230$ K [5]. We investigated the ab-plane and the ac-plane. The lattice constants at $T = 0.1$ K are $a = 8.160$ Å, $b = 5.067$ Å $c = 10.24$ Å.

Figure 1 shows the neutron intensity of $CeCu_{5.5}Au_{0.5}$ along $(h\,0\,0)$ at $T = 0.05$ K. Besides the nuclear reflections at integer positions, additional incommensurate scattering occurs. These magnetic Bragg peaks are resolution limited. The wave vector can be described by $q = (\pm 0.59, 0, 0)$. $q_h = 0.590 \pm 0.005$ can be approximated by 10/17. These incommensurate reflections disappear at temperatures higher than 1 K, in good agreement with the Néel temperature known from specific heat and susceptibility measurements [4]. The reflections at (1 0 0) and (3 0 0), appearing at forbidden nuclear positions are temperature independent and therefore not connected to the magnetic transition. The smallest magnetic wave vector $q_0 = (0.59, 0, 0)$ corresponds to the strongest

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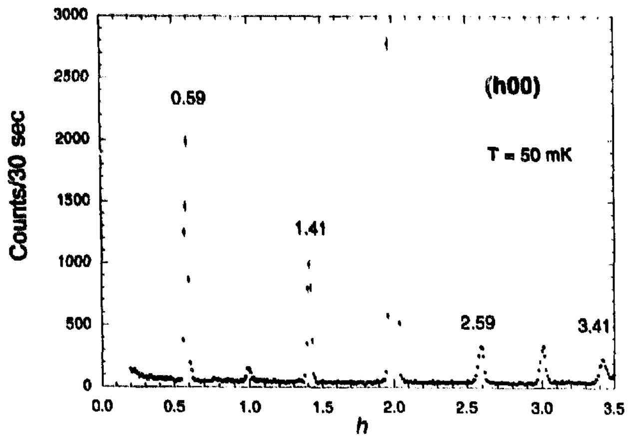

Fig. 1. $(h\,0\,0)$ scan of $CeCu_{5.5}Au_{0.5}$ at low temperature $T = 50$ mK.

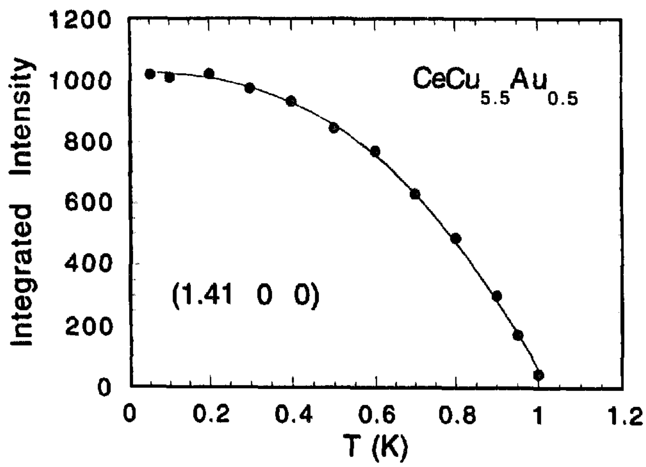

Fig. 2. Integrated intensity of the magnetic reflection at $q = (1.41\,0\,0)$ versus temperature T. The line is a guide to the eye.

reflection observed in the powder data at $q = 0.44$ Å^{-1} [3]. Also, the other reflections of the powder can be completely identified by higher zone reflections of the same q-value as $(2 - 0.59, 0, 0)$ and $(1 + 0.59, 1, 1)$. A scan along $(0\,k\,0)$ did not show any additional temperature-dependent scattering. This suggests that this q_0 is the only independent wave vector describing the magnetic order in this compound. Therefore the wave vectors of the correlations in $CeCu_6$ $(0\,0.85\,0)$ and $(1\,0\,0)$ [1] are not present in the ordered phase of $CeCu_{5.5}Au_{0.5}$. The wave vector along a^* changes from commensurate, describing fluctuations in $CeCu_6$, to incommensurate, describing long-range magnetic order in the "diluted" compound $CeCu_{5.5}Au_{0.5}$.

Figure 2 displays the temperature dependence of one magnetic reflection, (1.41, 0, 0). The integrated intensity of the sample rotation is shown versus temperature. Radial scans performed at several temperatures confirm that the incommensurate wave vector remains unchanged. The intensity increases monotonically towards lower temperatures, finally saturating for $T < 0.2$ K. The whole curve can be well described by $I = I_0\,(1 - (T/T_N)^{5/2})$ as a guide to the eye with $T_N = 1.02$ K.

To get a complete picture of the magnetic structure of $CeCu_{5.5}Au_{0.5}$ we measured several magnetic reflections in both planes. No significant angular dependence could be observed in the ab-plane, whereas the intensities of the magnetic reflections in the ac-plane show a strong angular dependence, which confirms that the direction of the magnetic moment is along the c-axis, as already suggested by the magnetization data [4]. The q-dependence can be approximated by $f^2 = \exp\{-(q/a_f)^2\}$ with $a_f = 2.8$ Å^{-1}, which is a bit smaller than the theoretical value for Ce^{3+}, $a_f = 4.3$ Å^{-1} [6]. Other harmonics of this incommensurate wave vector of observable intensity could not be found. Therefore, these data are consistent with magnetic moments oriented along the c-axis with a linear incommensurate sinusoidal modulation along the a-direction. This implies a strong modulation of moment size for two adjacent Ce ions, but no evidence for a circular wave is found here in this anisotropic [4] compound. The magnitude of the ordered moment can only be obtained reliably by a thorough analysis of the nuclear reflections, which is difficult due to the complex crystal structure of $CeCu_{5.5}Au_{0.5}$ at low temperatures. A rough estimate for the proposed incommensurate structure would yield a moment of $\sim 1\,\mu_B$, somewhat larger than inferred from magnetization measurements [4].

In conclusion, neutron diffraction on a single crystal revealed the magnetic structure of the heavy fermion alloy $CeCu_{6-x}Au_x$ with $x = 0.5$, where the wave vector is different from that of the short-range correlations in $CeCu_6$. To check any change of this incommensurate structure with the Au concentration in the magnetic ordered regime of $CeCu_{6-x}Au_x$, further investigation near the critical x and also of $x = 1$, which is a chemically ordered ternary compound [7], is necessary.

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